Heat Transfer in a Gas Mixture between Two Parallel Plates: Finite-difference Analysis of the Boltzmann Equation

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Abstract. The problem of heat transfer and temperature distribution in a binary mixture of rarefied gases between two parallel plates with different temperatures is investigated on the basis of kinetic theory. Under the assumption that the gas molecules are hard spheres and undergo diffuse reflection on the plates, the Boltzmann equation is analyzed numerically by means of an accurate finite-difference method, in which the complicated nonlinear collision integrals are computed efficiently by the deterministic numerical kernel method. As a result, the overall quantities (the heat flow in the mixture, etc.) as well as the profiles of the macroscopic quantities (the molecular number densities of the individual components, the temperature of the total mixture, etc.) are obtained accurately for a wide range of the Knudsen number. At the same time, the behavior of the velocity distribution function is clarified with high accuracy.

INTRODUCTION

The problem of heat transfer and temperature distribution in a rarefied gas between two parallel plates with different temperatures is one of the classical problems in rarefied gas dynamics, and a large number of theoretical and experimental works have been devoted to this problem, especially in the case of single-component gases (see, e.g., [1–4] and the references cited in [3,4]). Early theoretical works covering a wide range of the Knudsen number were mainly based upon either moment and variational methods, containing arbitrary assumptions on the form of the velocity distribution function, or numerical analysis using model Boltzmann equations. Only in 1989, Ohwada *et al.* [3] reported an accurate numerical solution of the linearized Boltzmann equation for a hard-sphere gas in the case of a small temperature difference between the plates. Their solution method was a finite-difference method, in which the collision integral was computed efficiently as well as accurately by the numerical kernel method developed by Sone *et al.* [5]. Subsequently, Ohwada extended the method to the collision integral of the full Boltzmann equation in his shock-structure analysis [6] and then applied it to the heat-transfer problem for a nonsmall temperature difference between the plates [4,7].

As for the case of binary gas mixtures, the accumulation of the results is not satisfactory, though some analyses (by means of a moment method) as well as experiments were performed in 1970's [8,9]. In the present study, therefore, we investigate the heat-transfer problem for a binary mixture of hard-sphere gases on the basis of the full Boltzmann equation for a large temperature difference, aiming to provide an accurate numerical solution that can be regarded as a standard for the problem. Recently, the present authors have extended Ohwada's numerical kernel method for the nonlinear collision integral to the case of binary mixtures in their study of shock wave structure [10]. The same method is employed in the present analysis.

PROBLEM

Consider a rarefied mixture of two gases, say components A and B, in the domain $0 \leq X_1 \leq D$ between two parallel plane walls at rest, where X_i is a rectangular coordinate system in space. Let the wall at $X_1 = 0$ be kept at temperature T_I and that at $X_1 = D$ at temperature T_{II}. Investigate the steady behavior of the mixture (temperature distribution, heat flow, etc.) on the basis of kinetic theory under the following assumptions:

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14. ABSTRACT
The problem of heat transfer and temperature distribution in a binary mixture of rarefied gases between two parallel plates with different temperatures is investigated on the basis of kinetic theory. Under the assumption that the gas molecules are hard spheres and undergo diffuse reflection on the plates, the Boltzmann equation is analyzed numerically by means of an accurate finite-difference method, in which the complicated nonlinear collision integrals are computed efficiently by the deterministic numerical kernel method. As a result, the overall quantities (the heat flow in the mixture, etc.) as well as the profiles of the macroscopic quantities (the molecular number densities of the individual components, the temperature of the total mixture, etc.) are obtained accurately for a wide range of the Knudsen number. At the same time, the behavior of the velocity distribution function is clarified with high accuracy.

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(i) The molecules of each component are hard spheres, and the interaction between two gaseous molecules is the complete elastic collision.
(ii) The molecules of each component are reflected according to the diffuse reflection condition on the walls.

BASIC EQUATION

Let $\boldsymbol{\xi} = (\xi_1, \xi_2, \xi_3)$ be the molecular velocity and $F^\alpha(X_1, \boldsymbol{\xi})$ the velocity distribution function of the molecules of α-component ($\alpha = A, B$). The Boltzmann equation in the present problem is written as

$$\xi_1 \frac{\partial F^\alpha}{\partial X_1} = \sum_{\beta=A,B} J^{\beta\alpha}(F^\beta, F^\alpha), \qquad (\alpha = A, B), \tag{1}$$

$$J^{\beta\alpha}(f, g) = [(d_m^{\beta\alpha})^2/2] \int [f(\boldsymbol{\xi}_*^{\beta\alpha}) g(\boldsymbol{\xi}^{\beta\alpha}) - f(\boldsymbol{\xi}_*) g(\boldsymbol{\xi})] |\mathbf{e} \cdot \boldsymbol{V}| d\Omega d\boldsymbol{\xi}_*, \tag{2}$$

$$\boldsymbol{\xi}^{\beta\alpha} = \boldsymbol{\xi} + \frac{\mu^{\beta\alpha}}{m^\alpha}(\mathbf{e} \cdot \boldsymbol{V})\mathbf{e}, \quad \boldsymbol{\xi}_*^{\beta\alpha} = \boldsymbol{\xi}_* - \frac{\mu^{\beta\alpha}}{m^\beta}(\mathbf{e} \cdot \boldsymbol{V})\mathbf{e}, \quad \boldsymbol{V} = \boldsymbol{\xi}_* - \boldsymbol{\xi}, \tag{3}$$

$$d_m^{\beta\alpha} = (d_m^\alpha + d_m^\beta)/2, \qquad \mu^{\beta\alpha} = 2m^\alpha m^\beta/(m^\alpha + m^\beta). \tag{4}$$

Here, m^α and d_m^α are the mass and diameter of a molecule of α-component; $\boldsymbol{\xi}_*$ is the integration variable for $\boldsymbol{\xi}$, $\mathbf{e}$ is a unit vector, $d\boldsymbol{\xi}_* = d\xi_{*1} d\xi_{*2} d\xi_{*3}$, and $d\Omega$ is the solid-angle element around $\mathbf{e}$; the domain of integration is the whole space of $\boldsymbol{\xi}_*$ and all directions of $\mathbf{e}$.

The boundary condition on the walls ($X_1 = 0$ and D) is expressed as follows: For $\boldsymbol{\xi} \cdot \boldsymbol{n} > 0$,

$$F^\alpha(X_1, \boldsymbol{\xi}) = \sigma_w^\alpha \Big(\frac{m^\alpha}{2\pi k T_w}\Big)^{3/2} \exp\Big(-\frac{m^\alpha |\boldsymbol{\xi}|^2}{2kT_w}\Big), \qquad \sigma_w^\alpha = -\Big(\frac{2\pi m^\alpha}{kT_w}\Big)^{1/2} \int_{\boldsymbol{\xi}_* \cdot \boldsymbol{n} < 0} \boldsymbol{\xi}_* \cdot \boldsymbol{n} F^\alpha(X_1, \boldsymbol{\xi}_*) d\boldsymbol{\xi}_*, \tag{5}$$

where

$$T_w = T_I, \quad \boldsymbol{n} = (1, 0, 0), \quad \text{at } X_1 = 0, \quad \text{and} \qquad T_w = T_{II}, \quad \boldsymbol{n} = (-1, 0, 0), \quad \text{at } X_1 = D, \tag{6}$$

and k is the Boltzmann constant.

If we rewrite the equation and boundary condition in a dimensionless form, we find that the problem is characterized by the following five parameters: m^B/m^A, d_m^B/d_m^A, T_{II}/T_I, n_{av}^B/n_{av}^A, and Kn. Here, n_{av}^α is the average molecular number density of α–component in the domain $0 \le X_1 \le D$, and Kn$= l_0/D$ is the Knudsen number, where $l_0 = [\sqrt{2}\pi (d_m^A)^2 n_{av}]^{-1}$ is the mean free path of the molecules of A–component when it is in the equilibrium state at rest with number density $n_{av} = n_{av}^A + n_{av}^B$.

NUMERICAL ANALYSIS

We first note that in the present problem we can seek the solution in the form $F^\alpha(X_1, \xi_1, \eta)$, where $\eta = (\xi_2^2 + \xi_3^2)^{1/2}$. We analyze Eqs. (1)–(6) numerically by means of an iterative finite-difference method. The key

TABLE 1. Heat flow $q_i = (q_1, 0, 0)$ of the total mixture for $T_{II}/T_I = 2$. Here, $p_0 = k n_{av} T_I$ is the reference pressure.

		$m^B/m^A = 0.5$, $d_m^B/d_m^A = 1$		$m^B/m^A = 0.25$, $d_m^B/d_m^A = 0.5$	
n_{av}^B/n_{av}^A	Kn	$q_1/[p_0(2kT_I/m^A)^{1/2}]$	Δ (%)	$q_1/[p_0(2kT_I/m^A)^{1/2}]$	Δ (%)
0.1	0.1	−0.184	0.45	−0.207	0.72
0.1	1	−0.509	0.19	−0.547	0.19
0.1	10	−0.656	0.049	−0.693	0.047
1	0.1	−0.209	0.34	−0.370	0.67
1	1	−0.589	0.15	−0.814	0.13
1	10	−0.763	0.047	−0.966	0.036
10	0.1	−0.245	0.34	−0.659	0.19
10	1	−0.677	0.10	−1.124	0.075
10	10	−0.871	0.038	−1.244	0.014

issue in the analysis is an accurate and efficient computation of the complicated collision integral $J^{\beta\alpha}$ using the discrete values F^{α}_{ijl} of F^{α} at the grid points $(X_1^{(i)}, \xi_1^{\alpha(j)}, \eta^{\alpha(l)})$ in the (X_1, ξ_1, η) space. For this purpose, we expand F^{α} at $X_1 = X_1^{(i)}$ as

$$F^{\alpha}(X_1^{(i)}, \xi_1, \eta) = \exp\Big(-\frac{(\bar{\eta}^{\alpha})^2}{2}\Big) \sum_{j,l} a_{jl}^{\alpha(i)} \Psi_j^{\alpha}(\bar{\xi}_1^{\alpha}) L_l((\bar{\eta}^{\alpha})^2), \qquad \bar{\xi}_1^{\alpha} = \xi_1 \Big(\frac{2kT_I}{m^{\alpha}}\Big)^{-\frac{1}{2}}, \quad \bar{\eta}^{\alpha} = \eta \Big(\frac{2kT_I}{m^{\alpha}}\Big)^{-\frac{1}{2}}, \quad (7)$$

where $\Psi_j^{\alpha}(\bar{\xi}_1^{\alpha})$ is a localized basis function that is sectionally quadratic, takes unity at $\bar{\xi}_1^{\alpha} = \xi_1^{\alpha(j)}(2kT_I/m^{\alpha})^{-1/2}$, and is nonzero only in its neighborhood; $L_l(y)$ is the Laguerre polynomial in y of order l. The coefficients $a_{jl}^{\alpha(i)}$ are determined in such a way that Eq. (7) coincides with F_{ijl}^{α} at the grid point $(\xi_1^{\alpha(j)}, \eta^{\alpha(l)})$. If we substitute Eq. (7) into the collision integral $J^{\beta\alpha}(F^{\beta}, F^{\alpha})$, it is expressed as a linear combination of the collision integrals for the functions of the form $(\bar{\eta}^{\alpha})^{2m}\Psi_n^{\alpha}$. The latter collision integrals are independent of F_{ijl}^{α} and therefore can be computed beforehand (numerical collision kernel). Once the numerical kernel is prepared, the computation of the collision integral in each iteration step is reduced to simple products and sums of matrices. In this way, high efficiency in the computation of the collision integral is attained (see [6,10] for the details).

RESULT OF ANALYSIS

The computation was carried out for $T_{II}/T_I = 2$, $(m^B/m^A,\ d_m^B/d_m^A) = (0.25, 0.5)$ and $(0.5, 1)$, $n_{av}^B/n_{av}^A = 0.1$, 1, and 10, and Kn= 0.1, 1, and 10. To show the result, we denote by n^{α} the molecular number density of α–component ($\alpha = A, B$) and by T and $q_i = (q_1, 0, 0)$ the temperature and the heat flow of the total mixture, respectively [i.e., $n^{\alpha}=\int F^{\alpha} d\boldsymbol{\xi}$, $(3knT,\ 2q_1)=\int(1,\ \xi_1)|\boldsymbol{\xi}|^2(m^A F^A + m^B F^B)d\boldsymbol{\xi}$, where $n = n^A + n^B$ and $d\boldsymbol{\xi}=d\xi_1 d\xi_2 d\xi_3$]. Note that the flow velocity of each component vanishes identically and the heat flow q_1 is independent of X_1 in the present problem because of the conservation of mass and that of energy.

The values of q_1 in all the cases are shown in Table 1, where $p_0 = kn_{av}T_I$ is a reference pressure. The numerical result of q_1 varies slightly with X_1 because of numerical error. Its average, say q_{1av}, over $0 \le X_1 \le D$ is shown as q_1 in the table. The maximum variation of q_1 over $0 \le X_1 \le D$ relative to q_{1av}: $\Delta = \max|q_1 - q_{1av}|/|q_{1av}|$, which gives a good measure of accuracy of the computation, is shown in percentage in Table 1. Figure 1–3 show the profiles of the number densities n^A and n^B and of the temperature T for the case of $m^B/m^A = 0.25$, $d_m^B/d_m^A = 0.5$: Fig. 1 is for $n_{av}^B/n_{av}^A = 0.1$, Fig. 2 for $n_{av}^B/n_{av}^A = 1$, and Fig. 3 for $n_{av}^B/n_{av}^A = 10$. The smaller molecules (the molecules of B–component) have a larger mean free path. Since Kn is based on the average number density of the total mixture and on the diameter of the larger molecules (the molecules of A–component), the effective Knudsen number at the same Kn is larger for larger values of n_{av}^B/n_{av}^A. Therefore, the temperature jump on the walls at the same Kn is larger for larger n_{av}^B/n_{av}^A. In Figs. 1–3, the

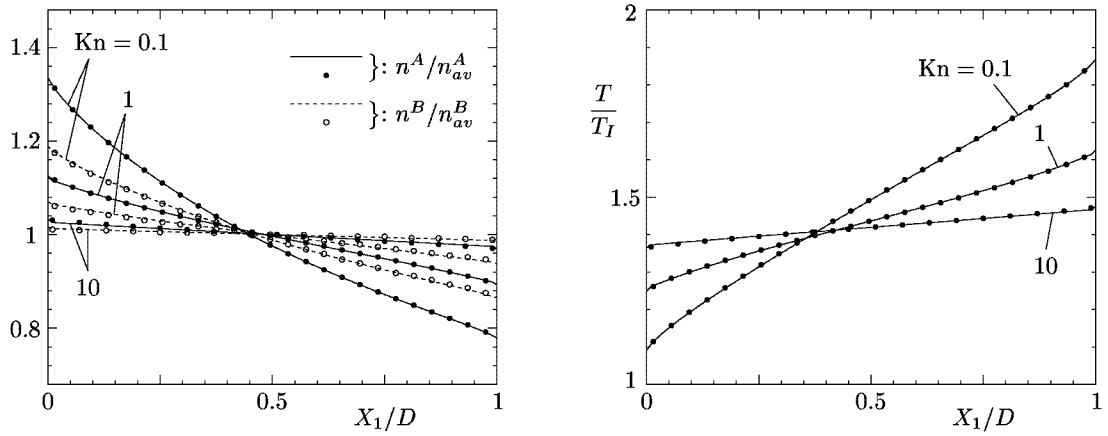


FIGURE 1. Profiles of the number densities n^A and n^B and of the temperature of the total mixture T for $m^B/m^A = 0.25$, $d_m^B/d_m^A = 0.5$, and $n_{av}^B/n_{av}^A = 0.1$. Here, — and --- indicate the result by the finite-difference method, and • and ○ that by the DSMC method.

corresponding result obtained by the direct simulation Monte Carlo (DSMC) method [11] is also shown for comparison. The DSMC result shows good agreement with the finite-difference result.

The velocity distribution functions F^α at two points near the walls in the cases corresponding to Figs. 1–3 are shown in Figs. 4–6, respectively. That is, F^α at $\eta(2kT_I/m^A)^{-1/2} = 0.15$ and 1.35 are shown as functions of ξ_1. In the case of free-molecular gas (Kn $= \infty$), the velocity distribution functions for any X_1 are discontinuous at $\xi_1 = 0$. For large Kn (Kn $= 10$), though the discontinuity vanishes because of the molecular collision, the gradient near $\xi_1 = 0$ is still very steep. The change around $\xi_1 = 0$ becomes milder as the Knudsen number decreases. The corresponding result by the DSMC method is also shown in Figs. 4–6.

The data about grid systems are summarized here. Let us put $c_I^A = (2kT_I/m^A)^{1/2}$. We divided the interval $0 \le X_1 \le D$ into 100 uniform sections for Kn= 1 and 10 and into 100 nonuniform sections (minimum size $4 \times 10^{-6}D$ at $X_1 = 0$ and D; maximum size $0.0294D$ at $X_1 = D/2$) for Kn= 0.1. We used uniform grids for ξ_1: For Kn= 0.1 and 1, the grid size is $0.15c_I^A$ and the range is restricted to $-6c_I^A \le \xi_1 \le 6c_I^A$ ($m^B/m^A = 0.5$) or $-8.7c_I^A \le \xi_1 \le 8.7c_I^A$ ($m^B/m^A = 0.25$) for A–component and to $-8.4c_I^A \le \xi_1 \le 8.4c_I^A$ ($m^B/m^A = 0.5$) or $-12c_I^A \le \xi_1 \le 12c_I^A$ ($m^B/m^A = 0.25$) for B–component; for Kn= 10, the grid size is $0.106c_I^A$ and the range is restricted to $-5.73c_I^A \le \xi_1 \le 4.45c_I^A$ ($m^B/m^A = 0.5$) or $-7.85c_I^A \le \xi_1 \le 6.58c_I^A$ ($m^B/m^A = 0.25$) for A–component and to $-7.85c_I^A \le \xi_1 \le 6.58c_I^A$ ($m^B/m^A = 0.5$) or $-10.82c_I^A \le \xi_1 \le 9.55c_I^A$ ($m^B/m^A = 0.25$) for B–component. For η, we used nonuniform 14 grid points defined by $(2kT_I/m^\alpha)^{1/2}\sqrt{y_k}$ ($\alpha = A, B$) for Kn= 0.1 and 1 and $(2kT_I/m^\alpha)^{1/2}\sqrt{y_k/2}$ for Kn= 10, where y_k ($k = 1, ..., 14$) are the zeros of the Laguerre polynomial $L_{14}(y)$ (see [10]).

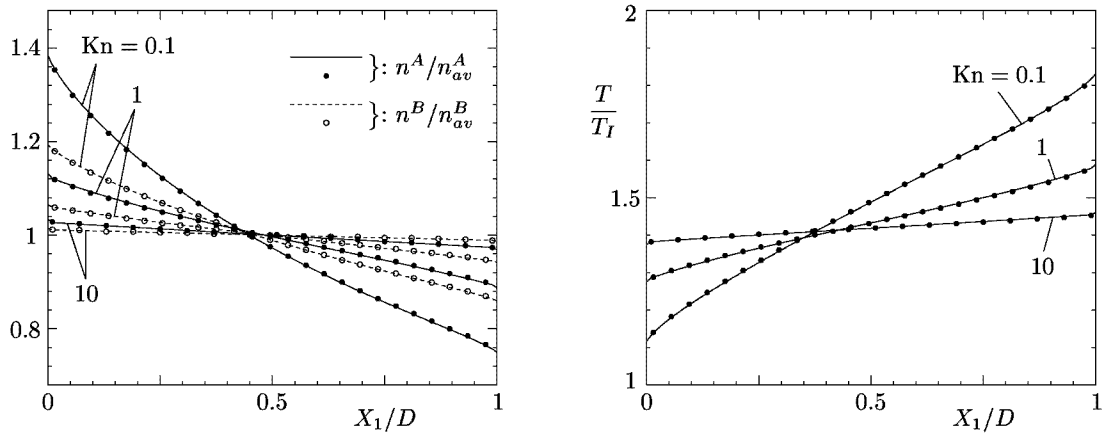


FIGURE 2. Profiles of the number densities n^A and n^B and of the temperature of the total mixture T for $m^B/m^A = 0.25$, $d_m^B/d_m^A = 0.5$, and $n_{av}^B/n_{av}^A = 1$. See the caption of Fig. 1.

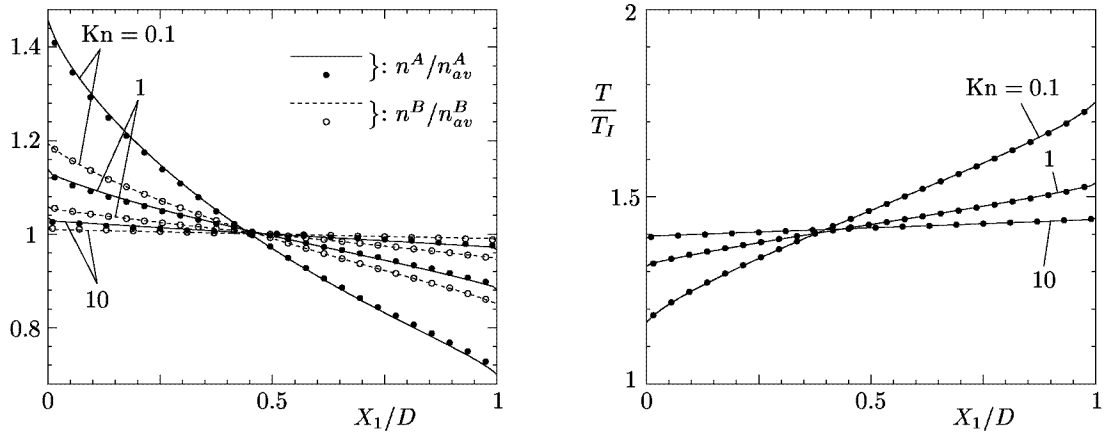
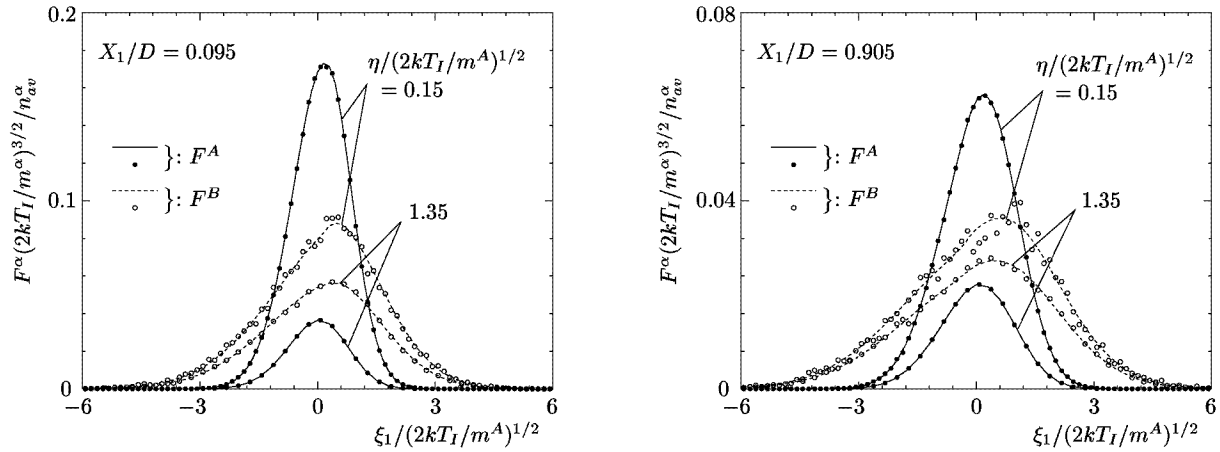
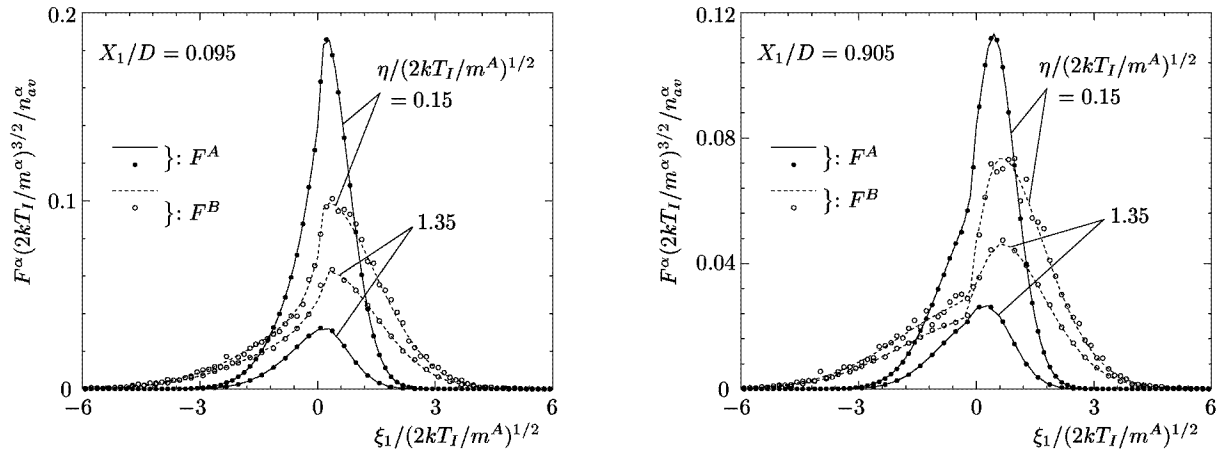


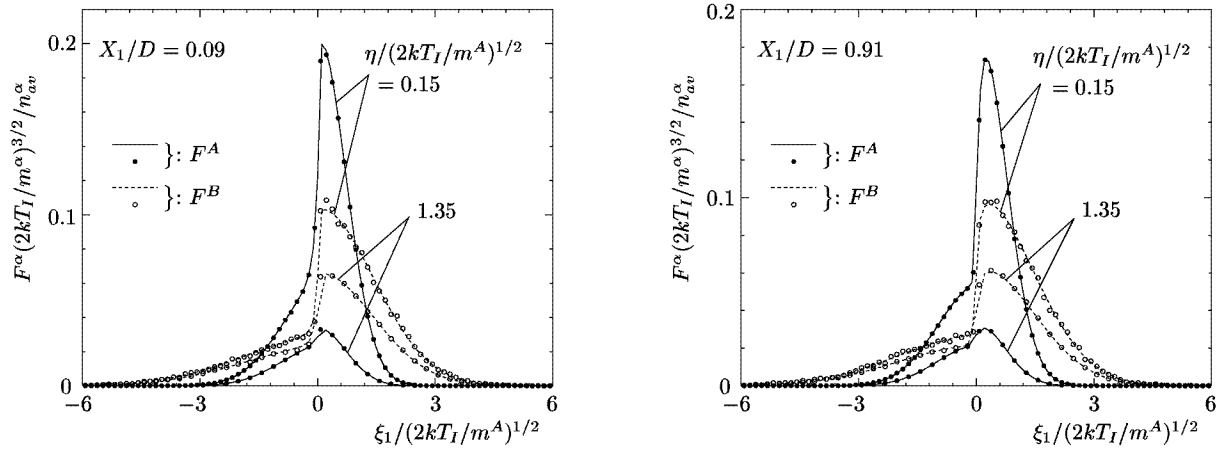
FIGURE 3. Profiles of the number densities n^A and n^B and of the temperature of the total mixture T for $m^B/m^A = 0.25$, $d_m^B/d_m^A = 0.5$, and $n_{av}^B/n_{av}^A = 10$. See the caption of Fig. 1.



(a) Kn = 0.1

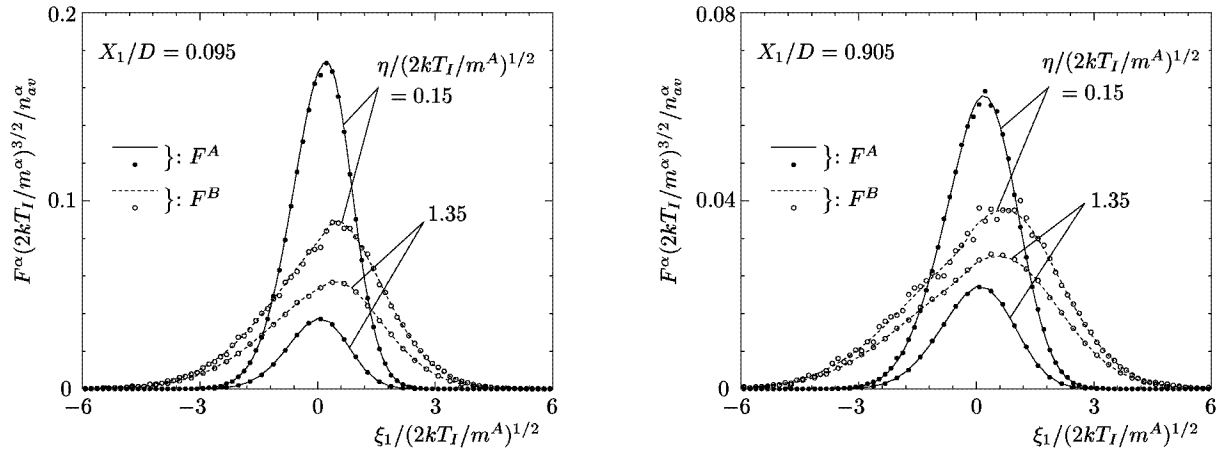


(b) Kn = 1

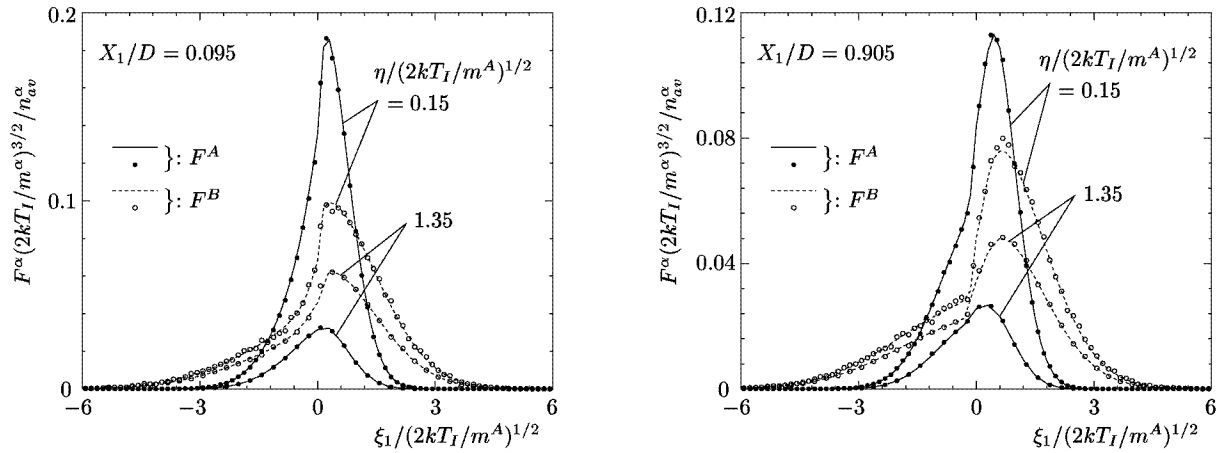


(c) Kn = 10

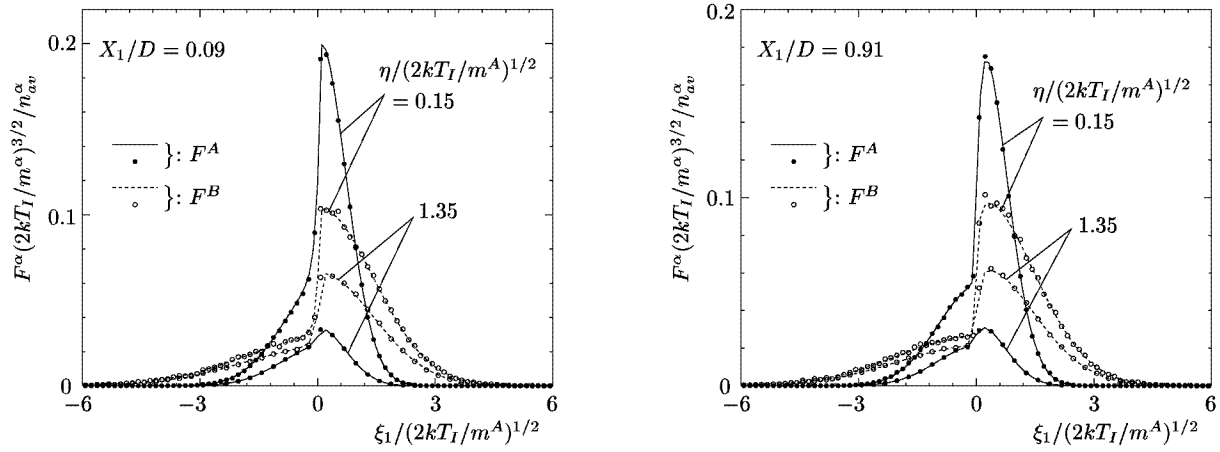
FIGURE 4. Velocity distribution functions F^A and F^B at two points near the walls for $m^B/m^A = 0.25$, $d^B_m/d^A_m = 0.5$, and $n^B_{av}/n^A_{av} = 0.1$ (cf. Fig. 1). (a) Kn = 0.1, (b) Kn = 1, (c) Kn = 10. Here, — and --- indicate the result by the finite-difference method, and • and ○ that by the DSMC method. The F^α at $X_1/D = 0.095$ and 0.905 are shown in (a) and (b), while F^α at $X_1/D = 0.09$ and 0.91 are shown in (c).



(a) Kn = 0.1

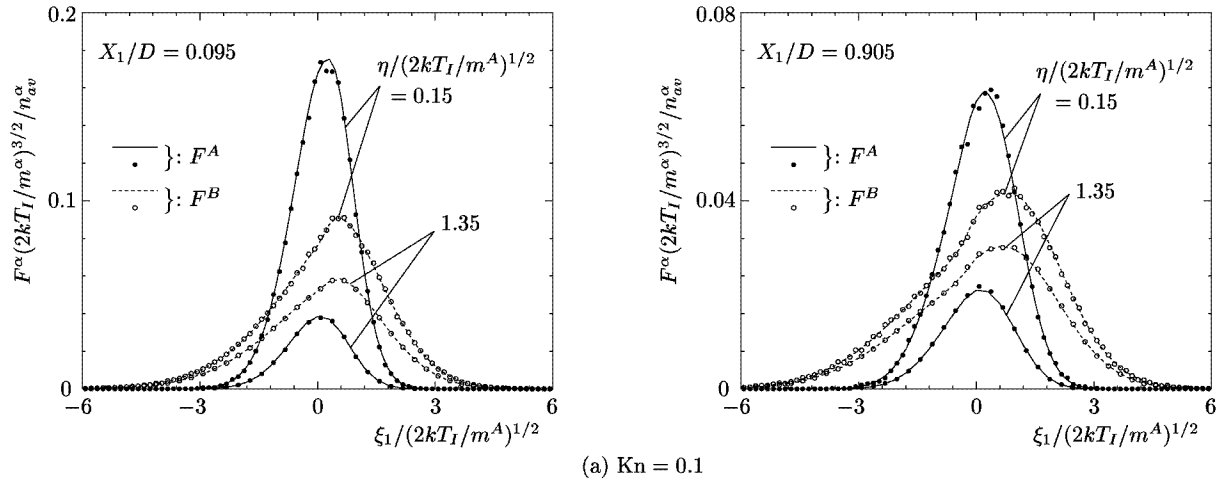


(b) Kn = 1

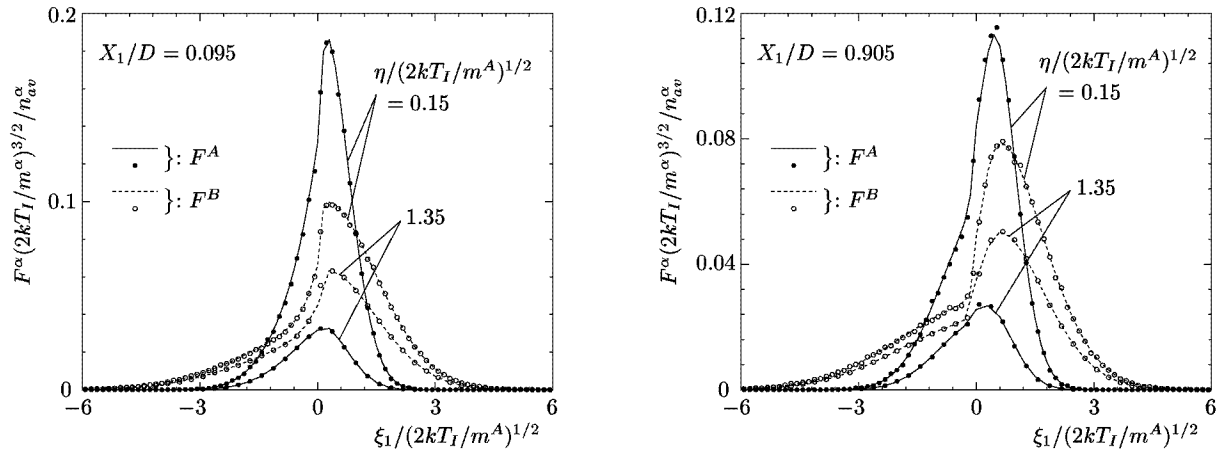


(c) Kn = 10

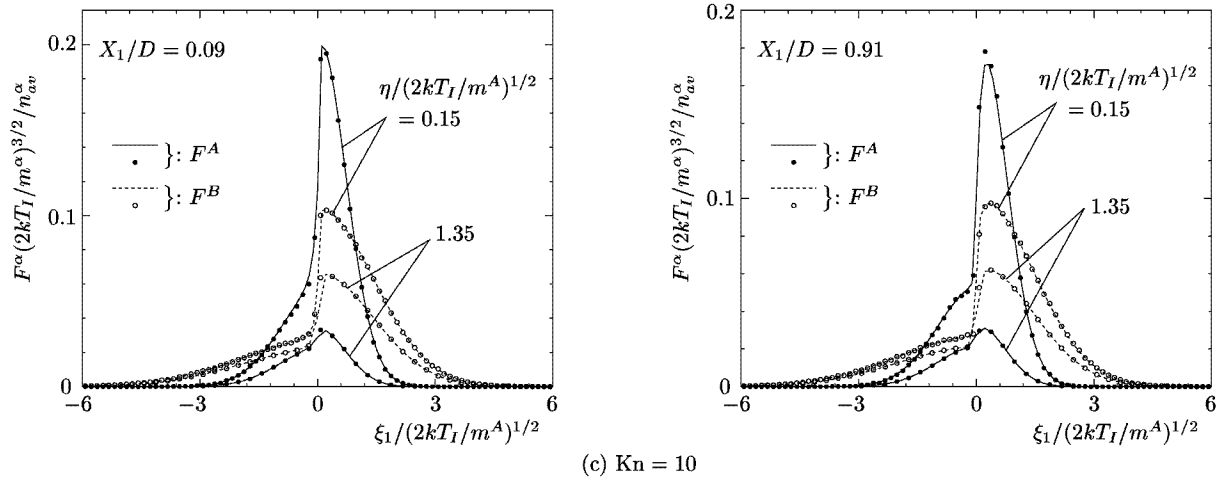
FIGURE 5. Velocity distribution functions F^A and F^B at two points near the walls for $m^B/m^A = 0.25$, $d^B_m/d^A_m = 0.5$, and $n^B_{av}/n^A_{av} = 1$ (cf. Fig. 2). (a) Kn = 0.1, (b) Kn = 1, (c) Kn = 10. See the caption of Fig. 4.



(a) Kn = 0.1



(b) Kn = 1



(c) Kn = 10

FIGURE 6. Velocity distribution functions F^A and F^B at two points near the walls for $m^B/m^A = 0.25$, $d^B_m/d^A_m = 0.5$, and $n^B_{av}/n^A_{av} = 10$ (cf. Fig. 3). (a) Kn = 0.1, (b) Kn = 1, (c) Kn = 10. See the caption of Fig. 4.

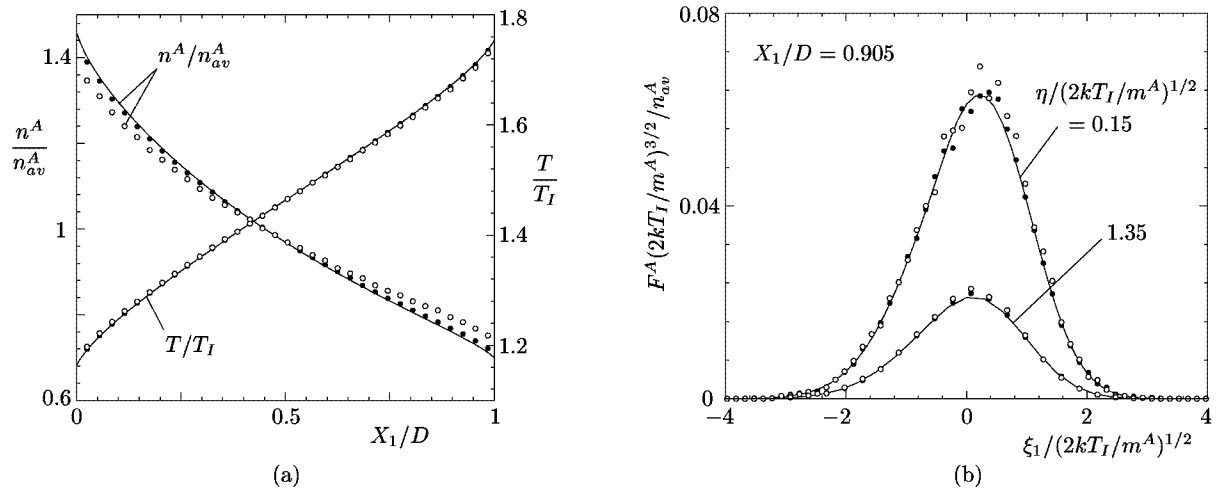


FIGURE 7. DSMC computations with two different numbers of simulation particles for $m^B/m^A = 0.25$, $d^B_m/d^A_m = 0.5$, Kn = 0.1, and $n^B_{av}/n^A_{av} = 10$. (a) Number density n^A and temperature T (cf. Fig. 3). (b) Velocity distribution function F^A at $X_1/D = 0.905$ (cf. Fig. 6). Here, — indicates the finite-difference result, ○ the DSMC result with $(N^A, N^B) = (25, 250)$, and • that with $(N^A, N^B) = (100, 1000)$.

Finally, we give information about the DSMC computational system. We used 50 (Kn = 10) or 100 (Kn = 0.1, 1) uniform cells in the interval $0 \le X_1 \le D$. Let N^α be the average number of simulation particles per cell for α–component. Then, (N^A, N^B)=(1000, 100) for $n^B_{av}/n^A_{av} = 0.1$, (250, 250) for $n^B_{av}/n^A_{av} = 1$, and (100, 1000) for $n^B_{av}/n^A_{av} = 10$ [(N^A, N^B)=(2000, 200) for $n^B_{av}/n^A_{av} = 0.1$ and (200, 2000) for $n^B_{av}/n^A_{av} = 10$ in the case of $m^B/m^A = 0.25$, $d^B_m/d^A_m = 0.5$, and Kn = 10]. The average of 2×10^4 samples taken at each 50 time steps is shown in Figs. 1–6. For small or large n^B_{av}/n^A_{av}, the total number of simulation particles increases because sufficient particles are necessary for the component with smaller number density (the same weight is used for both components in the present computation). We also carried out the DSMC computation with fewer particles, an example of which is shown in Fig. 7. That is, the result with (N^A, N^B)=(25, 250) of the case $m^B/m^A = 0.25$, $d^B_m/d^A_m = 0.5$, Kn = 0.1, and $n^B_{av}/n^A_{av} = 10$ is shown in the figure, together with the result with (N^A, N^B)=(100, 1000). Although it is smooth, the profile of n^A with (N^A, N^B)=(25, 250) deviates recognizably from that by the finite-difference method [Fig. 7(a)].

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